

Reaction dynamics of $\text{P}(^4\text{S}) + \text{O}_2(\text{X } ^3\Sigma^-) \rightarrow \text{O}(^3\text{P}) + \text{PO}(\text{X } ^2\Pi)$ on a global CHIPR potential energy surface of $\text{PO}_2(\text{X } ^2\text{A}_1)$: implication for atmospheric modelling

Guangan Chen¹, Zhi Qin^{*12}, Ximinng Li¹, Linhua Liu^{*123}

¹School of Energy and Power Engineering, Shandong University, 250061, Jinan, China.

²Optics and Thermal Radiation Research Center, Institute of Frontier and Interdisciplinary Science, Shandong University, 266237, Qingdao, China

³School of Energy Science and Engineering, Harbin Institute of Technology, 150001, Harbin, China

Correspondence to: Zhi Qin (z.qin@sdu.edu.cn) and Linhua Liu (liulinhua@sdu.edu.cn)

S1 Supplement of TDWP calculations

Table S1 displays the parameters used in the TDWP calculations. The J -shifting method was used in the calculation and the reaction probabilities of $J = 0$ to 270 were obtained.

Table S1 Parameters used in the TDWP calculations. All parameters are given in atomic units, except for the numbers of quantities or indicated otherwise.

Parameter	Value
Scattering coordinate (R) range	0.01-13
Number of translational basis functions	450
Internal coordinate (r) range	1.6-9.6
Number of vibrational basis functions	285
Number of rotational basis functions	150
Absorption region length in R / r	3.0 / 3.0
Absorption strength in R / r	0.03 / 0.03
Center of initial wave packet on scattering coordinate	9.5
K-block	2
Propagation time	50000
Time step for propagation	10

S2 Supplement of fitting rate constants

The constant rate constants of TDWP ($v = 0, j = 0$), QCT ($v = 0, j = 0$) and QCT (Thermal) for the $\text{P}(^4\text{S}) + \text{O}_2(\text{X } ^3\Sigma^-) \rightarrow \text{O}(^3\text{P}) + \text{PO}(\text{X } ^2\Pi)$ reaction can be approximated using the three-parameter Kooij function (within 1 per cent), which is expressed as

$$k(T) = A \left(\frac{T}{300} \right)^\alpha e^{-\beta/T} \quad (\text{S1})$$

where A , α , and β are fitting parameters. The rate constant curves are divided into four temperature ranges, and the fitting parameters are summarized in Table S2. The fitted rate constants deviate less than 1 per cent from our calculated ones.

Table S2 Parameters according to Kooij function for the rate constants.

Method	T / K	$A / \text{cm}^3\text{s}^{-1}$	α	β / K
TDWP ($v = 0, j = 0$)	200 - 600	2.2508×10^{-12}	1.3554	1041.9940
	600 - 1000	4.4682×10^{-12}	0.9430	1283.2565
	1000 - 2000	8.6398×10^{-12}	0.6532	1596.5685
	2000 - 5000	6.7105×10^{-11}	-0.0146	3193.4739
QCT (Thermal)	200 - 600	4.7988×10^{-13}	2.5132	734.5248
	600 - 1000	6.7196×10^{-12}	0.7068	1574.9928
	1000 - 2000	6.7933×10^{-12}	0.7215	1610.7254
	2000 - 5000	2.0656×10^{-12}	1.0844	590.6460
QCT ($v = 0, j = 0$)	2000 - 5000	5.7104×10^{-11}	0.0244	3237.2285